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Quantum Calisthenics: Gaussians, The Path Integral and Guided Numerical Approximations

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It is apparent to anyone who thinks about it that, to a large degree, the basic concepts of Newtonian physics are quite intuitive, but quantum mechanics is not. My purpose in this talk is to introduce you to a new, much more intuitive way to understand how quantum mechanics works. I refer to this method as a guided numerical approximation scheme and it is based upon a new look at what the path integral tells us about states in Hilbert space. I begin with simple exactly solvable models and show how to handle problems which cannot be dealt with analytically, this includes the treatment of the evolution of a Gaussian wave-packet in an anharmonic potential as well tunneling problems (i.e., instanton effects)

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[†] The animations referred to in the text can be viewed by going to $http:\backslash\backslash slac.stanford.edu\backslash\sim niv$ and following the link to the animations for Quantum Calisthenics

1. Quantum Mechanics Isn't Intuitive !

It is apparent to anyone who thinks about it that, to a large degree, the basic concepts of Newtonian physics are quite intuitive, but quantum mechanics is not. My purpose in this talk is to introduce you to a new, much more intuitive way to understand how quantum mechanics works.

I begin with an incredibly easy way to derive the time evolution of a Gaussian wave-packet for the case free and harmonic motion without any need to know the eigenstates of the Hamiltonian. This discussion is completely analytic and I will later use it to relate the solution for the behavior of the Gaussian packet to the Feynman path-integral and stationary phase approximation. It will be clear that using the information about the evolution of the Gaussian in this way goes far beyond what the stationary phase approximation tells us.

Next, I introduce the concept of the *bucket brigade approach* to dealing with problems that cannot be handled totally analytically. This approach combines the intuition obtained in the initial discussion, as well as the intuition obtained from the path-integral, with simple numerical tools. My goal is to show that, for any specific process, there is a simple Hilbert space interpretation of the stationary phase approximation. I will then argue that, from the point of view of numerical approximations, the trajectory obtained from my generalization of the stationary phase approximation specifies that subspace of the full Hilbert space that is needed to compute the time evolution of the particular state under the full Hamiltonian. The prescription I will give is totally non-perturbative and we will see, by the grace of Maple animations computed for the case of the anharmonic oscillator Hamiltonian, that this approach allows surprisingly accurate computations to be performed with very little work. To view these animations go to $http:\backslash\backslash slac.stanford.edu\backslash\sim niv$. I think of this approach to the path-integral as defining what I call a *guided numerical approximation scheme*.

After the discussion of the anharmonic oscillator I will turn to tunneling problems and show that the *instanton* can also be though of in the same way. I will do this for the classic problem of a double well potential in the extreme limit when the splitting between the two lowest levels is extremely small and the tunneling rate from one well to another is also very small.

2. Gaussian Wavefunctions and the Path Integral

Discussions of one-dimensional quantum mechanics usually begin by considering the space of square integrable functions $\psi(x)$ on the interval $-\infty < x < \infty$. This space of functions is acted upon two operators, $\mathbf{p}$ and $\mathbf{x}$, where the action of these operators on a state $\psi(x)$ is defined to be

$$\mathbf{x}\,\psi(x) = x\psi(x) \tag{2.1}$$

$$\mathbf{p}\,\psi(x) = \frac{1}{i}\frac{d\psi}{dx}(x); \tag{2.2}$$

i.e., $\mathbf{x}$ is simply multiplication by the variable x and $\mathbf{p}$ is differentiation with respect to the variable x. Given these definitions it is simple to show that $\mathbf{x}$ and $\mathbf{p}$ satisfy the commutation relation

$$[\mathbf{x},\mathbf{p}] = i. \tag{2.3}$$

In what follows we will devote a great deal of attention to the properties of Gaussian wave-packets. For our purpose a Gaussian packet of width $1/\sqrt{\gamma}$ is defined as the solution to the equation

$$(i\mathbf{p} + \gamma\mathbf{x})\psi(x) = 0. \tag{2.4}$$

To show this is the same as the usual condition is simple, but worth doing explicitly since we will use it over and over again. The steps are

$$(\frac{d\psi}{dx}(x)+\gamma\psi(x))=0 \tag{2.5}$$

$$\psi(x)=Ce^{-\frac{1}{2}x^2} \tag{2.6}$$

where constant C is determined by the normalization condition

$$\int_{-\infty}^{\infty}dx\,\psi^*(x)\,\psi(x)=1, \tag{2.7}$$

that means that $C=\left(\frac{\gamma}{\pi}\right)^{1/4}$.

From this point on we will write a Gaussian satisfying this equation by the symbol $|0_\gamma\rangle$.

3. Shifted Gaussians

In what follows it will be important for us to consider Gaussian wave-packets centered about points $\tilde{x}\neq 0$; i.e., Gaussian packets shifted away from the origin. As is customary, these packets will be constructed by applying the operator

$$U(\tilde{x})=e^{-i\mathbf{p}\tilde{x}}=\sum_{i=0}^{\infty}\frac{(-i)^n}{n!}\mathbf{p}^n\tilde{x}^n \tag{3.1}$$

to the state $|0_\gamma\rangle$ to obtain the state $|\tilde{x}_\gamma\rangle$; where $\tilde{x}$ is an arbitrary number and $\mathbf{p}$ is the momentum operator.

To see that this operation does what we want observe that

$$e^{-i\mathbf{p}\tilde{x}}\mathbf{x}e^{i\mathbf{p}\tilde{x}} = \mathbf{x}-i\tilde{x}[\mathbf{p},\mathbf{x}]+\frac{(-i)^2}{2!}\tilde{x}^2\,[\mathbf{p},[\mathbf{p},\mathbf{x}]]+\ldots \tag{3.2}$$

$$= \mathbf{x}-\tilde{x} \tag{3.3}$$

where all but the first two terms of the expansion vanish since the commutator of $\mathbf{p}$ with $\mathbf{x}$ is proportional to the unit operator. Thus,

$$e^{-i\mathbf{p}\tilde{x}}(i\mathbf{p}+\gamma\mathbf{x})\,|0_\gamma\rangle = 0, \tag{3.4}$$

$$e^{-i\mathbf{p}\tilde{x}}(i\mathbf{p}+\gamma\mathbf{x})\,e^{i\mathbf{p}\tilde{x}}\,(e^{-i\mathbf{p}\tilde{x}}\,|0_\gamma\rangle) = 0, \tag{3.5}$$

$$e^{-i\mathbf{p}\tilde{x}}(i\mathbf{p}+\gamma\mathbf{x})\,e^{i\mathbf{p}\tilde{x}}\,|\tilde{x}_\gamma\rangle = 0. \tag{3.6}$$

Now observe that $\mathbf{p}$ commutes with $U(\tilde{x})$ so that Eq.3.6 becomes

$$(i\mathbf{p}+\gamma(x-\tilde{x}))|\tilde{x}_\gamma\rangle=0. \tag{3.7}$$

Using the previous argument, thinking of $|\tilde{x}_\gamma\rangle$ as a function of x, we have

$$|\tilde{x}_\gamma\rangle=\left(\frac{\gamma}{\pi}\right)^{1/4}e^{-\frac{\gamma}{2}(x-\tilde{x})^2}. \tag{3.8}$$

This, of course, is what we wished to show.

I have only included this elementary discussion to show how one can manipulate the equation that defines a Gaussian packet in order to obtain a useful result. In the next section I will use the same sort of argument to derive the evolution in time of an arbitrary Gaussian packet.

4. Evolution of a Gaussian With Free Hamiltonian

The operator form of the time-dependent Schrodinger equation, given a Hamiltonian **H**, says that the state $|\psi(t)\rangle$ satisfies the equation

$$\frac{d}{dt}|\psi(t)\rangle = -i\mathbf{H}\,|\psi(t)\rangle. \tag{4.1}$$

As is well known, the solution to this equation is

$$|\psi(t)\rangle = e^{-it\mathbf{H}}\,|\psi(t)\rangle. \tag{4.2}$$

To derive the time evolution of a Gaussian packet we multiply Eq. 2.4 by e^{-itH}, where H is defined to be

$$H = \frac{\mathbf{p}^2}{2m}, \tag{4.3}$$

for some mass m; i.e., we consider

$$e^{-it\frac{\mathbf{p}^2}{2m}}\,(i\mathbf{p}+\gamma\mathbf{x})\,|0_\gamma\rangle \;=\; 0 \tag{4.4}$$

$$e^{-it\frac{\mathbf{p}^2}{2m}}\,(i\mathbf{p}+\gamma\mathbf{x})\,e^{it\frac{\mathbf{p}^2}{2m}}\,|0_\gamma(t)\rangle \;=\; 0 \tag{4.5}$$

$$(i\mathbf{p}(t)+\gamma\mathbf{x}(t))\,|0_\gamma(t)\rangle \;=\; 0; \tag{4.6}$$

where the time dependent operators $\mathbf{x}(t)$ and $\mathbf{p}(t)$ are

$$\mathbf{x}(t) \;=\; e^{-it\,\frac{\mathbf{p}^2}{2m}}\,\mathbf{x}\,e^{it\frac{\mathbf{p}^2}{2m}} = \mathbf{x} - t\,\frac{\mathbf{p}}{m}, \tag{4.7}$$

$$\mathbf{p}(t) \;=\; e^{-it\,\frac{\mathbf{p}^2}{2m}}\,\mathbf{p}\,e^{it\frac{\mathbf{p}^2}{2m}} = \mathbf{p}. \tag{4.8}$$

These results follow from the definition of the exponential and the commutation relations. Substituting this into Eq. 4.6 we obtain

$$(i\mathbf{p}+\gamma(\mathbf{x}-\frac{t}{m}\,\mathbf{p})|0_\gamma(t)\rangle \;=\; 0 \tag{4.9}$$

$$\left(\left(1+\frac{i\gamma t}{m}\right)\,i\mathbf{p}+\gamma\mathbf{x}\right)\,|0_\gamma(t)\rangle \;=\; 0 \tag{4.10}$$

$$(i\mathbf{p}+\gamma(t)\mathbf{x})\,|0_\gamma(t)\rangle \;=\; 0. \tag{4.11}$$

This, as we have already shown, means

$$|0_\gamma(t)\rangle = C(t)\;e^{-\frac{1}{2}\,\gamma(t)x^2}, \tag{4.12}$$

where

$$\gamma(t) = \frac{\gamma}{1+i\frac{\gamma t}{m}}. \tag{4.13}$$

The fact that

$$C(t) = \left(\frac{\gamma}{\pi}\right)^{1/4}\,\frac{1}{\sqrt{1+i\frac{\gamma t}{m}}} \tag{4.14}$$

follows directly from the equation

$$\frac{d}{dt}(C(t)e^{-\frac{1}{2}\gamma(t)x^2}) = -iC(t)\,\frac{d^2}{dx^2}e^{-\frac{1}{2}\gamma(t)x^2}), \tag{4.15}$$

which is simply a differential equation for $\ln(C(t))$. I have bothered to include the entire derivation of the time-dependent wave-function to show how powerful manipulating the defining equation for the Gaussian packet can be. Because the time dependent packet drops off as $e^{-\frac{1}{2}\gamma(t)x^2}$ where $\gamma(t)$ is complex, we will refer to this as a generalized Gaussian packet. An animation showing how this wave-function looks as it evolves in time is shown at the beginning of the html file that I referred to previously this paper. It is followed by animations showing how different coherent states evolve using the free Hamiltonian.

5. The Harmonic Oscillator

Now that we have the exact solution of the time evolution of an arbitrary Gaussian packet under the free Hamiltonian, let us consider the next simplest case, the harmonic oscillator Hamiltonian; i.e.

$$H = \frac{\mathbf{p}^2}{2m} + \frac{m\,\omega^2}{2}\mathbf{x}^2. \tag{5.1}$$

Once again if we start by multiplying the defining equation of a Gaussian packet by the exponential of H we find

$$e^{-itH}\ (i\,\mathbf{p} + \gamma\mathbf{x})\ |0_\gamma\rangle = 0, \tag{5.2}$$

or

$$(i\,\mathbf{p}(t) + \gamma\mathbf{x}(t))|0_\gamma(t)\rangle = 0, \tag{5.3}$$

where the time-dependent operators $\mathbf{p}(t)$ and $\mathbf{x}(t)$ are defined to be

$$\mathbf{p}(t) = e^{-itH}\,\mathbf{p}\,e^{itH} \qquad \text{and} \qquad \mathbf{x}(t) = e^{-itH}\,\mathbf{x}\,e^{itH}. \tag{5.4}$$

It follows immediately from this equation and the commutation relations of $\mathbf{p}$ and $\mathbf{x}$ that

$$\frac{d\mathbf{x}}{dt} = \frac{1}{m}\mathbf{p}(t) \qquad \text{and} \qquad \frac{d\mathbf{p}}{dt} = -\omega^2\,\mathbf{x}(t). \tag{5.5}$$

Since this is simply a first order differential equation with the boundary conditions $\mathbf{p}(t=0) = \mathbf{p}$ and $\mathbf{x}(t=0) = \mathbf{x}$, it has the unique solution

$$\mathbf{x}(t) \;=\; \cos(\omega t)\,\mathbf{x} + \frac{1}{m\,\omega}\sin(\omega t)\mathbf{p} \tag{5.6}$$

$$\mathbf{p}(t) \;=\; \cos(\omega t)\,\mathbf{p} - m\,\omega\sin(\omega t)\mathbf{x} \tag{5.7}$$

Substituting these into Eq. 5.3 we obtain, as before,

$$\left(i\mathbf{p} + \gamma\left(\frac{\cos(\omega t) + \frac{im\omega}{\gamma}\ \sin(\omega t)}{\cos(\omega t) + \frac{i\gamma}{m\omega}\ \sin(\omega t)}\right)\ \mathbf{x}\right)\ |0_\gamma(t)\rangle = 0 \tag{5.8}$$

Thus we see that the evolution of a Gaussian packet in a harmonic oscillator potential is once again a generalized Gaussian with a $\gamma(t)$ that is periodic in time. Note, if and only if $\gamma = m\,\omega$, the packet doesn't change in time and it is simply multiplied by a phase $e^{-it\,\omega/2}$; i.e. when $\gamma = m\,\omega$ the packet is an eigenstate of the harmonic oscillator Hamiltonian.

6. Coherent States

Previously we discussed Gaussians shifted to a mean position $\tilde{x}$. Now we will generalize the shifted state to one that has a non-vanishing expectation value for both **x** and **p**; i.e., consider the time evolution of the state

$$e^{-i\mathbf{p}\tilde{x}+i\tilde{p}\mathbf{x}}\,|0_\gamma\rangle \tag{6.1}$$

This is called a coherent state.

Clearly, using the previous arguments, multiplying this state to the left by e^{-itH} we obtain

$$e^{-i\mathbf{p}(t)\tilde{x}+i\tilde{p}\mathbf{x}(t)}\,|0_\gamma(t)\rangle. \tag{6.2}$$

Collecting terms this can be rewritten as

$$e^{-i\mathbf{p}\tilde{x}_{\rm class}(t)+i\tilde{p}_{\rm class}(t)\mathbf{x}}\,|0_\gamma(t)\rangle. \tag{6.3}$$

where $|0_\gamma(t)\rangle$ was calculated in the preceding section and $\tilde{x}_{\rm class}(t)$ and $\tilde{p}_{\rm class}(t)$ are the solutions to the classical equations of motion for a particle moving in a harmonic potential that initially is located at the position $\tilde{x}$ with momentum $\tilde{p}$. It is not an accident that this is the same trajectory one would obtain by doing the stationary phase approximation to the path integral. To make the analogy between the formula for the propagation of an arbitrary shifted Gaussian and the stationary phase approximation more striking let us rewrite Eq. 6.3 as

$$e^{i\tilde{p}_{\rm class}(t)\tilde{x}_{\rm class}(t)}\;e^{-i\mathbf{p}\tilde{x}_{\rm class}(t)+i\tilde{p}_{\rm class}(t)(\mathbf{x}-\tilde{x}_{\rm class}(t))}\,|0_\gamma(t)\rangle. \tag{6.4}$$

This form of the generalized Gaussian packet shows that the packet center moves along the classical trajectory for a particle starting with the given initial mean position and mean momentum. Furthermore, it shows that, if we write the position dependent phase factor that gives the shifted packet the correct mean classical momentum, so that it has the value one at the packet center, then the entire packet is multiplied by a time dependent phase factor that is the exponential of the classical action. These results are also what is seen in derivations of the path-integral using coherent states with a single fixed value for γ. What is not captured in the coherent state derivation of the path-integral is the fact that γ changes in time and, in fact, becomes complex. This is why that approach is less powerful than what I will do next.

7. The Bucket-Brigade Approach to the Path-Integral

We now understand how a generalized Gaussian packet propagates with the free or harmonic oscillator Hamiltonian. Now, let us spend a few moments connecting this knowledge to the usual derivation of the path integral using Gaussian coherent states. Most derivations begin by rewriting the time evolution operator as a product of the evolution operator for many small time steps and inserting a complete set of states between each term in the product;i.e.,

$$\langle\gamma_{\rm final}|e^{-it\mathbf{H}}|\gamma_{\rm init}\rangle = \langle\gamma_{\rm final}|\ldots|\gamma_{j+1}\rangle\langle\gamma_{j+1}|e^{-it\mathbf{H}/n}|\gamma_j\rangle\langle\gamma_j|e^{-it\mathbf{H}/n}|\gamma_{j-1}\rangle\langle\gamma_{j-1}|\ldots|\gamma_{\rm init}\rangle. \tag{7.1}$$

In Feynman's derivation of the path integral this complete set of states are δ-functions of x or p, as appropriate. Later derivations used coherent states, since the shifted coherent states form an

over-complete basis in terms of which one can construct a resolution of the identity operator. In either case, after deriving this identity one customarily makes the *stationary phase approximation*, which in effect selects a single intermediate state at each step. In all of these cases, however, even for the exactly solvable cases of the free particle, or the harmonic oscillator, the states selected by this step are not good approximations to the true evolution. We have already seen that the correct evolution of a free particle or a particle in a harmonic oscillator potential is a generalized shifted Gaussian with a complex $\gamma(t)$. Obviously, if we insert these states as intermediate states then the stationary phase approximation would produce the exact answer. This observation almost brings us to the formulation of the *bucket-brigade* approach to dealing with the Schrodinger equation. The missing step is the observation that as the number of steps in the decomposition of the evolution operator increases the number of states selected by the stationary phase approximation increases too. However, since these states are not orthogonal to one another, the number of significantly linearly independent states doesn't grow in the same way. To be more precise, I define the notion of significantly linearly independent states as follows: let the integers M and N, with $M < N$ define two decompositions of the time interval in the decomposition. Let $|\gamma_i\rangle$ and $|\psi_j\rangle$ be the two sets of states defined by the corresponding stationary phase condition, i.e. let them be the generalized Gaussian packets obtained by exactly propagating the initial state a time t/M or t/N. The larger set of states will not be significantly linearly independent of the smaller set if all of the larger states can be represented to some pre-defined accuracy as a linear combination of the smaller set of states.

Since dividing the time interval over which the evolution is occurring into ever smaller slices does not lead to increasing numbers of significantly linearly independent states, it follows that one can describe the continuous time evolution of the initial state to arbitrary accuracy be restricting attention to a finite dimensional sub-space of the full Hilbert space. In this section I will show that this is the case for free and harmonic evolution. To be precise, I will show that in order to compute the states $e^{-it\mathbf{H}}|\gamma_0\rangle$ for all values of t between some t_{initial} and t_{final} to high accuracy it suffices to, given some discrete set of states $|\psi_n\rangle$, compute the truncated operators

$$H_{nm} = \langle\gamma_n|\mathbf{H}|\gamma_m\rangle \qquad \text{and} \qquad N_{nm} = \langle\gamma_n|\mathbf{N}|\gamma_m\rangle, \tag{7.2}$$

and then exponentiate the finite matrix H_{nm} after transforming it to the orthonormal basis defined by the $|\psi_n\rangle$'s. In the accompanying .html I show how well this works for various initial states evolving either under the free Hamiltonian or the harmonic oscillator Hamiltonian.

8. A Non-Trivial Example: The Anharmonic Oscillator

I have argued that the bucket-brigade idea says that, with no significant loss of accuracy, we can restrict attention to a relatively small subspace of Hilbert space to compute the continuous time evolution of a given packet, I will now show that the same is true for Hamiltonians for which the time evolution cannot be exactly computed. To show how this works let us begin by considering the case of the anharmonic oscillator; i.e., the system defined by the Hamiltonian

$$\mathbf{H} = \frac{\mathbf{p}^2}{2m} + \lambda\,\mathbf{x}^4. \tag{8.1}$$

We will start, as before, with a Gaussian packet defined by the equation

$$(i\mathbf{p} + \gamma\mathbf{x})\,|0_\gamma\rangle = 0. \tag{8.2}$$

Then, it follows that the time-evolved packet satisfies the equation

$$e^{-it\mathbf{H}}(i\mathbf{p}+\gamma\mathbf{x})\,|\gamma_0\rangle = 0, \tag{8.3}$$

or

$$(i\mathbf{p}(t)+\gamma\mathbf{x}(t))\,|\gamma(t)\rangle = 0, \tag{8.4}$$

where $\mathbf{x}(t)$ and $\mathbf{p}(t)$ are defined as in Eq. 4.8. It not possible, however, to compute $\mathbf{x}(t)$ or $\mathbf{p}(t)$ exactly. We can however non-perturbatively approximate the evolution of a state

$$|x_i, p_i, \gamma(t)\rangle = e^{-ix_i\mathbf{p}+ip_i\mathbf{x}}\,|0_{\gamma(t)}\rangle \tag{8.5}$$

by evolving it with the *effective quadratic Hamiltonian*

$$\begin{aligned}\mathbf{H}_{\rm eff}(x_i,p_i,\gamma(t)) &= \frac{(\mathbf{p}+p_i)^2}{2m} + \lambda\,\langle Re(\gamma(t))|\,\mathbf{V}(\mathbf{x}+x_i)\,|Re(\gamma(t))\rangle &(8.6)\\ &+ \lambda\,\langle Re(\gamma(t))|\,\frac{d}{d\mathbf{x}}\mathbf{V}(\mathbf{x}+x_i)\,|Re(\gamma(t))\rangle\,(\mathbf{x}-x_i) &(8.7)\\ &+ \lambda\,\langle Re(\gamma(t))|\,\frac{d^2}{d\mathbf{x}^2}\mathbf{V}(\mathbf{x}+x_i)\,|Re(\gamma(t))\rangle\,(\mathbf{x}-x_i)^2. &(8.8)\end{aligned}$$

Note that in order to guarantee that the Hamiltonian is hermitian the expectation values are computed for Gaussian packets where $\gamma(t)$ is replaced by a Gaussian with the same where $\gamma(t)$ is replaced by the real part of $\gamma(t)$. Thus, with this in mind we define the iterative procedure where we begin with a generalized Gaussian

$$|\psi_n\rangle = C_n\, e^{i\,p_n\,(x-x_n)}\, e^{-\frac{1}{2}\,\gamma_n\,(x-x_n)^2} \tag{8.9}$$

and evolve it with a quadratic Hamiltonian with the generic form

$$\mathbf{H}_{\rm eff} = \frac{(\mathbf{p}+p_n)^2}{2m} + V_n - F_n\,(x-x_n) + \frac{m\,\omega_n^2}{2}. \tag{8.10}$$

Applying the formulas we already derived for the evolution of a generalized Gaussian in a harmonic potential we see that we get a new generalized Gaussian of the form

$$|\psi_{n+1}\rangle = C_{n+1}\, e^{i\,p(\delta t)_{n+1}\,(x-(x_n+\tilde{x}(\delta t)_{n+1}))}\, e^{-\frac{\gamma_{n+1}}{2}\,(x-(x_n+\tilde{x}(\delta t)_{n+1}))^2} \tag{8.11}$$

where the quantities appearing in this equation are given by the formulas

$$C_{n+1} = C_n\,\frac{1}{\sqrt{\cos(\omega_n\,\delta t)+\frac{i\,\gamma_n}{m\,\omega_n}\,\sin(\omega_n\,t)}}\, e^{\frac{iF_n^2}{2\,m\,\omega_n^2}}\, e^{-i\frac{F_n}{m\,\omega_n^2}\,(p(\delta t)_{n+1}-p_n)}\, e^{i\mathbf{p}(\delta t)_{n+1}x(\delta t)_{n+1}}, \tag{8.12}$$

and

$$\begin{aligned}x(\delta t)_{n+1} &= \frac{F_n}{m\,\omega_n^2}\,(1-\cos(\omega_n\,\delta t)) + \frac{\mathbf{p}_n}{m\,\omega_n}\,\sin(\omega_n\delta t) &(8.13)\\ p(\delta t)_{n+1} &= \cos(\omega_n\,\delta t)\,p_n + \frac{F_n}{\omega_n}\,\sin(\omega_n\,\delta t) &(8.14)\\ \gamma_{n+1} &= \frac{\cos(\omega_n\,\delta t)+\frac{im\,\omega_n}{\gamma_n}\,\sin(\omega_n\,\delta t)}{\cos(\omega_n\,\delta t)+\frac{i\,\gamma_n}{m\,\omega_n}\,\sin(\omega_n\,\delta t)}. &(8.15)\end{aligned}$$

Note, that at the n^{th} step the Hamiltonian parameters, for the case of the anharmonic oscillator are defined by the equations

$$V_n = \lambda\, x_n^4 + \frac{3\lambda}{\gamma_n}\, x_n^4 + \frac{3\lambda}{4\gamma_n^2} \tag{8.16}$$

$$F_n = -4\lambda\, x_n^3 - \frac{6\lambda}{\gamma_n}\, x_n \tag{8.17}$$

$$\omega_n = \sqrt{\frac{12\lambda}{m}\, x_n^2 + \frac{6\lambda}{m\gamma_n}}. \tag{8.18}$$

One repeats this process again and again, recomputing the effective Hamiltonian at each stage, and obtains a basis for the truncated Hilbert space. To compute the continuous time evolution of the initial state we exponentiate the truncated Hamiltonian, obtained by computing the matrix elements of the exact Hamiltonian between these Gaussian packets. Since these are Gaussians, this is easy to do. The comparison of this approximate computation and the exact result obtained from a brute force numerical approximation is shown in the previously referred to html file. That file contains many animations showing how a free Gaussian packet evolves in time under various circumstances, as well as how a Gaussian in a harmonic potential evolves in time. It also contains animations that compare the evolution using discretized, *bucket-brigade* states to exact solutions, both for the exactly solvable systems, as well as for the anharmonic oscillator. You will see that, in all cases, the agreement between the real and imaginary part of the wave-fucntion for approximate and exact calculation is quite remarkable.

9. Tunneling and Instantons

The final issue I want to touch upon is tunneling, which is important both for problems related to tunneling between different minima of a potential, and to general problems of scattering from a non-square barrier.

Consider the Hamiltonian for a particle in a double-well potential

$$\mathbf{H} = \frac{1}{2m}\,\mathbf{p}^2 + \lambda\,(\mathbf{x}^2 - f^2)^2. \tag{9.1}$$

If we now attempt to find stationary Gaussians there will be two solutions, one in each well. As before the classical moments, $\tilde{p}$ of each solution must be set to zero. Next, as is shown in the .html file, the condition that the force, the expectation value of the derivative of the potential, vanish means that in the left-hand well the Gaussian is shifted slightly to the right of the minimum and in the right-hand well the Gaussian is shifted slightly to the left. The parameter γ for each of the Gaussian's doesn't evolve in time determines γ in terms of the appropriate expectation value of the second derivative of the potential. If we stop at this point the bucket-brigade approach would now determine the future behavior of the system by computing the matrix elements of the Hamiltonian between these two states and the metric formed by taking the overlaps of the two states. This result alone tells us that tunneling takes place. However, and that is what we now wish to study, it severely underestimates the tunneling rate when the mass is large and the wells are well separated.

The question is "what states do we have to add in order to compute the tunneling rate accurately ?". The answer is, of course, determined by the instanton calculation.

The key point is that in order to improve the energies of the two lowest states it suffices to apply the operator $e^{-t\mathbf{H}}$ to compute the effective Hamiltonian [1]-[2]-[3]

$$\mathbf{H}_{ij}(t) = \left[\langle\psi_i|e^{-t\mathbf{H}}|\psi_l\rangle\right]^{-1/2} \langle\psi_l|e^{-\frac{t}{2}\mathbf{H}}\mathbf{H}e^{-\frac{t}{2}\mathbf{H}}|\psi_m\rangle \left[\langle\psi_m|e^{-t\mathbf{H}}|\psi_j\rangle\right]^{-1/2}. \tag{9.2}$$

If we now follow the path integral procedure and divide the product up into a number of steps and insert a set of generalized Gaussian packets

$$e^{-i\mathbf{p}\tilde{x}(t)+i\tilde{p}(t)\mathbf{x}}|\gamma(t)\rangle \tag{9.3}$$

where $\tilde{p}(t)$ is chosen so that, as is always the case,

$$\tilde{p}(t) = \frac{1}{m}\frac{d\tilde{x}}{dt}(t), \tag{9.4}$$

and for simplicity $\gamma(t)$ is chosen to be a constant, then it follows that this contribution to the transition element is maximized if the function $\tilde{x}(t)$ satisfies the equation

$$\frac{d^2}{dt^2}\tilde{x}(t) = 4\lambda\tilde{x}(t)\left(\tilde{x}(t)^2 - f^2\right) \tag{9.5}$$

where $\tilde{x}(t) = -c_{\min}$ and $d\tilde{x}(t=0)/dt = 0$, and γ is chosen to be the same as that for the initial and final Gaussian packet. A picture of the solution and the discretized choice of a finite number of these states is shown in the appropriate section of the .html file.

If we assume, as before, that these are the correct states to use to compute the time evolution of the initial Gaussian we simply compute the truncated Hamiltonian and exponentiate it. The corresponding animations in the accompanying .html file show that this computation is remarkably accurate for the real and imaginary part of the wavefunction, as a function of time, as well as for the tunneling rate.

It is a straightforward matter to extend these ideas to field theory, however time and space preclude discussing this question at this time.

References

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